
ADAS702: Postprocessor - Autostructure > adf09 file

The code accesses intermediate data sets of energy levels, autoionization rates and radiative rates created by ADAS701. It re-organises and collects these data to generate tables of state resolved and metastable resolved dielectronic recombination coefficients according to ADAS data format *adf09*. The code handles both (LS) coupling and intermediate coupling (IC) data. The original background version of the code was (and is) known as ADASDR.

Background:

The ADAS701 (AUTOSTRUCTURE) code produces large amounts of LS and IC data that, in general, cannot be processed by hand. The transition probabilities are normally combined in many different ways depending on the resonant process that you wish to study - here it is dielectronic recombination. The program ADAS702 reads the standard rate files produced by ADAS701 (*ols* etc. but renamed as *o1*, *o2* etc. or *olsu* etc. renamed as *o1u*, *o2u* etc.) and processes them, eventually, to produce *adf09* files. The same program reads both LS or IC data, producing the LS or IC variant of *adf09* (see the specification the data format in chapter 6). It is natural and efficient to calculate, process and archive each core excitation $n \rightarrow n'$ separately (but summed over l, l'). Since (part of the) data for alternative core excitations are normally present, it is necessary to state the core excitation to be processed so as to avoid double or multiple counting. The program also requires information on the metastable states and the recombined parents. In the case of a $\Delta n = 0$ core excitation (e.g. $2s \rightarrow 2p$) use can, and should be, made of the observed target/core energies. Normally, no other user supplied data is necessary.

In addition to the large book keeping operation necessary to convert the raw AUTOSTRUCTURE data into an *adf09* file, the code also supplements this data (automatically) internally with hydrogenic radiative rates for stabilizing transitions between Rydberg states. It is much more efficient, and accurate enough, to do it here and leave AUTOSTRUCTURE to compute only those transitions from the Rydberg states into the (non-hydrogenic) core (in addition to the core rates of course). The code only checks the n -value of final decay states and so all l -values of a given recombined n should be included in the AUTOSTRUCTURE run.

Setting up the driver data set

Introduction: All user supplied data is free-formatted and namelisted. Formatted data from ADAS701 (AUTOSTRUCTURE) is expected in file *o1* or unformatted data in file *o1u*. The file *o1* is checked first, if non-empty then *o1u* is ignored. In general, more than one rate file is needed to cover even a single core excitation e.g. the *KLL* and *KLn* transitions would normally be calculated with separate ADAS701 runs. The files should then be made available as *o1* and *o2*, or *o1u* and *o2u* if unformatted. Or, it might be more efficient to separate out a calculation into two ADAS701 runs by parity say. Currently, a maximum of 4 files (*o1*, *o2*, *o3*, *o4* or *o1u*, *o2u*, *o3u*, *o4u*) can be processed by a single ADAS702 run to produce a single *adf09* file. The file *paper.txt* contains a terse summary of DR cross sections as a function of Rydberg n and l for the user to check for convergence and an estimate of the total rate coefficient from each metastable for the core excitation being processed. A small amount of control information is also written and is of no concern unless the program fails and then, hopefully, the corrective action necessary by the user is indicated.

Dataset:

The first four characters of line 1 MUST be /LS/ or /IC/ so as to denote the type of data being processed. The rest of line 1 is for comments.

Namelists:

ONE:

COREX='n-m' selects the core transition $n \rightarrow m$ to be processed, where n and m are the initial and final principal quantum numbers. The l -values need not and must

not be specified i.e. 'n-m' is 3 characters. The default is ' ', no restriction on core excitations. Thus COREX should be specified.

(This control variable is still under test. Historically, a variable JCFJ was used to restrict DR contributions to those autoionizing configurations that arose in the first JCFJ configurations of the original ADAS701-AUTOSTRUCTURE run. Whilst reliable, use of JCFJ does require the original configuration list to be suitably ordered and is it more easily confused by the novice user. JCFJ is still present in the namelist for now and can be used if problems are encountered with COREX. If COREX is used, the configurations numbers of the autoionizing configurations considered are written to file *paper.txt* as a check.)

NTAR1=Number of initial (metastable) target states.

NTAR2=Number of final resolved (parent) states.

The values of (2S+1) L (case /LS/) or 2J p 2S+1 L (case /IC/, where p, S and L are for labelling purposes only in *adf09* - p is the parity) follow free-formatted after Namelist TWO for the NTAR2 parent states. (The files TERMS and LEVELS produced following a suitable target run with ADAS701 can provide this data.)

TWO:

NECOR=0 (default) does nothing.

.gt.0, read NECOR calculated then experimental energies (in Rydbergs) relative to the ground. They follow the statistical weight information.

Various "correction" factors are available in this namelist which can be applied to the radiative or autoionization rates for one reason or another. These may be detailed in the future.

Example 1.

(Na-like target, term resolved).

```
/LS/ Na-like target, 2p->3l core excitations.
&ONE NTAR1=2 NTAR2=4 COREX='2-3' &END
&TWO &END
2 0 2 1 2 2 2 0
```

Note

Example 2.

(Li-like target, level resolved).

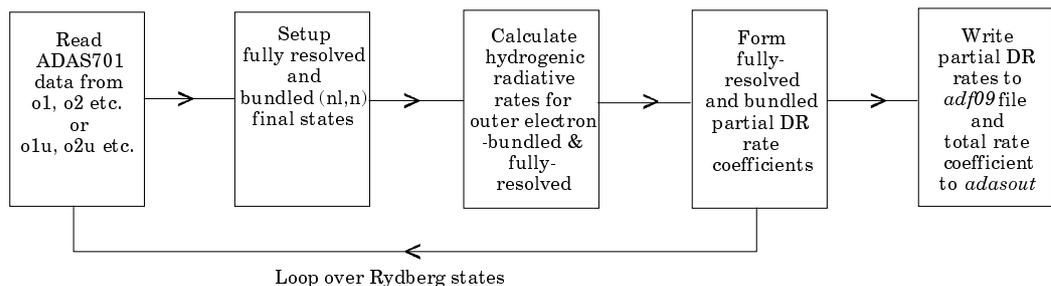
```
/IC/ Li-like target, 2s->2p core excitations.
&ONE NTAR1=1 NTAR2=3 COREX='2-2' &END
&TWO NECOR=3 &END
1 0 2 0
1 1 2 1
3 1 2 1
0.0 1.0311 1.0398 These are the calculated (core) energies for F6+.
0.0 1.0230 1.0319 These are observed. This text is not read.
```

Note

Program steps:

These are summarised in the schematic below.

Figure 8.2

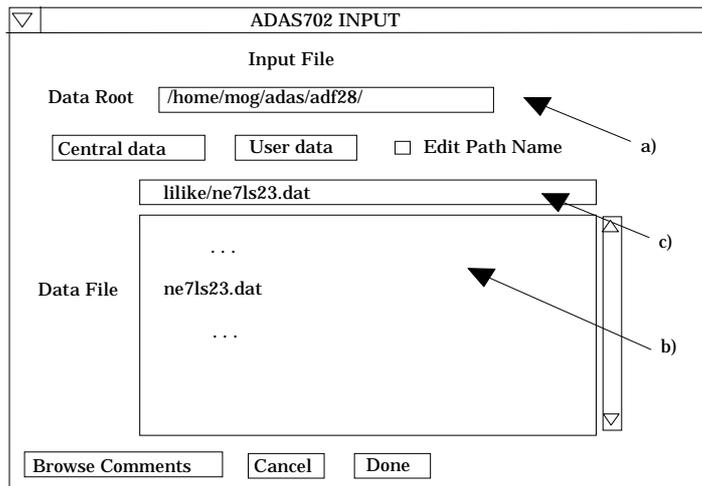


Interactive parameter comments:

There is no graphic output from this program. Initiate ADAS702 from the program selection menus in the usual manner.

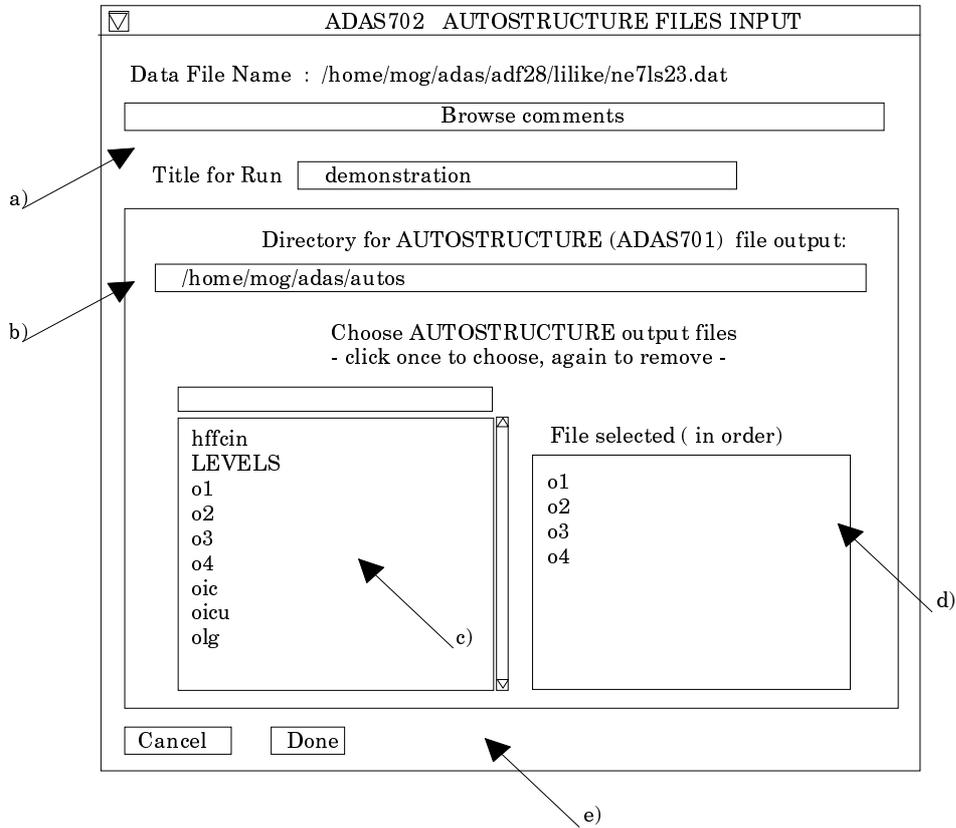
The **file selection window** has the appearance shown below

1. Data root a) shows the full pathway to the appropriate data subdirectories. The appropriate ADAS data format for input to this program is *adf28*. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility. It is expected that the user would prepare his/her own driver *adf28* data. Central ADAS of this type contains templates which can form the basis for creating one's own drivers.



2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
3. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
4. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
5. Once a data file is selected, the set of buttons at the bottom of the main window become active.
6. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what is broadly available in the dataset. The possibility of browsing the comments appears in the subsequent main window also.
7. Clicking the *Done* button moves you forward to the next window, which comprises a second stage of data file selection. Clicking the *Cancel* button takes you back to the previous window.
8. The second stage (AUTOSTRUCTURE output file selection) widget is shown below.
9. The name of the driver data set selected in the previous step is displayed at a) and its comments lines can be browsed by clicking the *Browse Comments* button. Also a title may be entered for the run in the text widget directly below.
10. Selection of the output files from the prior runs of ADAS701 (AUTOSTRUCTURE) which are required for post-processing are selected at b).

11. The default directory pathway is `./../<userid>adas/autos/` consistent with the default operation of ADAS701. The directory pathway is editable.
12. Available files for selection are shown in the scrollable selection window at c). Files generated by multiple runs of ADAS701 would normally be renamed as 'o1', 'o2' etc. or their unformatted versions 'o1u', 'o2u' etc. Click on a file to select it and click on it again to de-select. Selected files appear in the adjacent *Files selected* window at d). If more than four files are selected, a warning is issued. At least one file must be selected before the code will proceed.

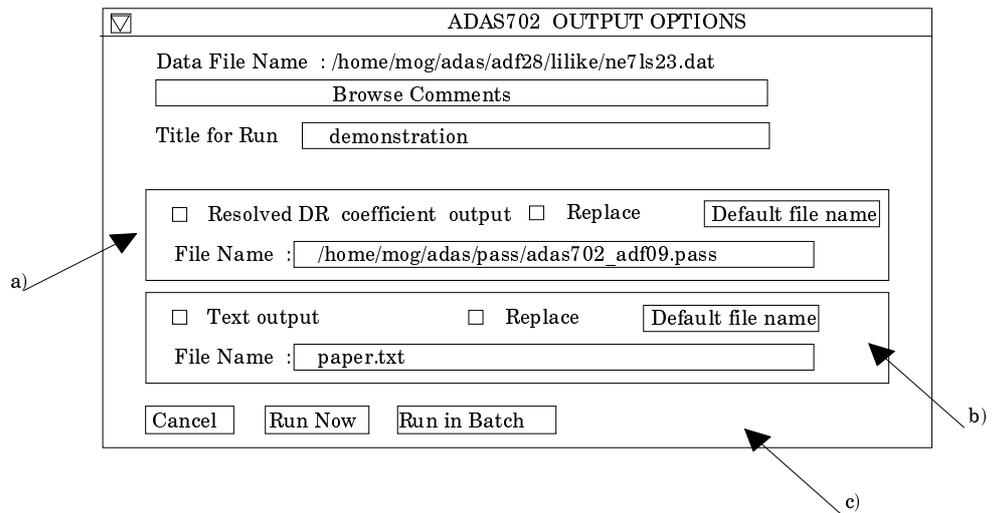


13. Click *Done* to advance to the *Output Options* screen in the usual manner.

There is no processing options window for ADAS702.

The **output options window** appearance is shown below

14. At a) output of the *adf09* file may be enabled. The *Default file name* and *Replace* options are available. By default, the output file is sent to your */pass* directory as `./../adas/pass/adas702_adf09.pass`.
15. At b) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated. **NB. It is essential to look at the *paper.txt* file to ensure that the code has operated as planned and hence that the resolved DR file (adf09) is valid.**



16. At the base of the window, the icon for *Exit to Menu* is present. This quits the program and returns you to the ADAS series 7 menu. Remember that *Done* takes you forward to the next screen while *Cancel* takes you back to the previous screen.

Illustration:

Notes: